

# Separability Probability Formulas and Their Proofs for Generalized Two-Qubit X-Matrices Endowed with Hilbert-Schmidt and Induced Measures

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## Abstract

Two-qubit X-matrices have been the subject of considerable recent attention, as they lend themselves more readily to analytical investigations than two-qubit density matrices of arbitrary nature. Here, we maximally exploit this relative ease of analysis to formally derive an exhaustive collection of results pertaining to the separability probabilities of generalized two-qubit X-matrices endowed with Hilbert-Schmidt and, more broadly, induced measures. Further, the analytical results obtained exhibit interesting parallels to corresponding earlier (but, contrastingly, not yet fully rigorous) results for general 2-qubit states—deduced on the basis of determinantal moment formulas. Geometric interpretations can be given to arbitrary positive values of the random-matrix Dyson-index-like parameter  $\alpha$  employed.

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## I. INTRODUCTION

In previous work [1, 2], the authors investigated the separability probabilities of  $4 \times 4$  density matrices ( $\rho$ ) with density approximation techniques [3] based on the moments of the determinant ( $|\rho^{PT}|$ ) of the partial transpose—the nonnegativity of which is necessary and sufficient for separability [4, 5]. The moment formulas employed involve a Dyson-index-like parameter  $\alpha$  which specializes to real, complex, quaternionic densities for  $\alpha = \frac{1}{2}, 1$  and  $2$ , respectively. As yet, the validity of the moment formulas is only a conjecture, but there is strong evidence that they are correct. By use of extraordinarily large ( $5 \times 10^{11}$  trials) Monte Carlo simulations, Fei and Joynt [6] obtained separability probability values agreeing to 4 decimal places with our results (cf. [7, 8]), that is  $\frac{29}{64}$ ,  $\frac{8}{33}$  and  $\frac{26}{323}$ , respectively. More generally still, we have also been investigating the general separability probability question [9] when  $k$ -th powers of the determinant ( $|\rho|$ ) times the Hilbert-Schmidt (HS) measure [10, 11]—that is, induced measure [10, 12, 13]—are used as the probability measure on the convex set of density matrices. Due to the extreme intractability of performing direct probability calculations by use of high-dimensional integration, these studies continue to be based on moment formulas and sophisticated numerical analysis (density approximation) techniques [3] to determine probabilities.

Recently, interesting results have been obtained for the subset of so-called X-matrices, which are a form of toy model for density matrices [7, 14, 15]. The present study exploits their simpler structure to directly, and now fully rigorously, compute the separability probabilities for the family of induced measures (including the particular [ $k = 0$ ] Hilbert-Schmidt case). Although the results obtained are numerically quite different from those [16] holding for the full, unrestricted matrices, they do exhibit a strong qualitative similarity. This can be taken as evidence that our earlier work [1, 2, 16] has been well directed. We note that in the X-matrix case, it has been possible to give geometric interpretations to arbitrary positive values of the Dyson-index-like parameter  $\alpha$ , not just integer and half-integer values, such as  $\frac{1}{2}$ ,  $1$  and  $2$  as described above (cf. [17]), and perhaps this idea can be extended to unrestricted sets of density matrices.

We start with the basic definitions. A  $4 \times 4$  X-density matrix  $\xi$  is positive semi-definite

with  $Tr(\xi) = 1$  and has the form

$$\xi = \begin{bmatrix} \xi_{11} & 0 & 0 & \xi_{14} \\ 0 & \xi_{22} & \xi_{23} & 0 \\ 0 & \overline{\xi_{23}} & \xi_{33} & 0 \\ \overline{\xi_{14}} & 0 & 0 & \xi_{44} \end{bmatrix};$$

the defining conditions are equivalent to  $\xi_{jj} \geq 0$  for  $1 \leq j \leq 4$ ,  $\xi_{14}, \xi_{23} \in \mathbb{C}$ ,  $\sum_{j=1}^4 \xi_{jj} = 1$ ,  $|\xi_{14}|^2 \leq \xi_{11}\xi_{44}$  and  $|\xi_{23}|^2 \leq \xi_{22}\xi_{33}$ . The partial transpose of  $\xi$  is denoted by  $\xi^{PT}$  and

$$\xi^{PT} = \begin{bmatrix} \xi_{11} & 0 & 0 & \xi_{23} \\ 0 & \xi_{22} & \xi_{14} & 0 \\ 0 & \overline{\xi_{14}} & \xi_{33} & 0 \\ \overline{\xi_{23}} & 0 & 0 & \xi_{44} \end{bmatrix}$$

Thus  $\det \xi^{PT} = (\xi_{11}\xi_{44} - |\xi_{23}|^2)(\xi_{22}\xi_{33} - |\xi_{14}|^2)$  and the density matrix  $\xi$  is separable if and only if  $\det \xi^{PT} \geq 0$ .

We induce a measure on the set  $\mathcal{X}$  of X-density matrices from the measure

$$\prod_{j=1}^4 d\xi_{jj} (r_5 r_6)^{2\alpha-1} dr_5 dr_6 d\theta_5 d\theta_6,$$

on the cone of all positive semi-definite X-matrices, where  $\xi_{14} = r_5 e^{i\theta_5}$ ,  $\xi_{23} = r_6 e^{i\theta_6}$  ( $r_j \geq 0$ ,  $-\pi < \theta_j \leq \pi$ ,  $j = 5, 6$ ). The details of normalizing the measure to be a probability measure appear later. We will show for any  $\alpha > 0$  that

$$\Pr \{ \det \xi^{PT} \geq 0 \} = p(\alpha) := \frac{1}{\sqrt{2\pi}} \frac{\Gamma(\alpha + \frac{1}{2})^2 \Gamma(\alpha + \frac{3}{2})}{\Gamma(\alpha + \frac{3}{4}) \Gamma(\alpha + 1) \Gamma(\alpha + \frac{5}{4})},$$

in particular,  $p(\frac{1}{2}) = \frac{16}{3\pi^2}$ ,  $p(1) = \frac{2}{5}$ ,  $p(2) = \frac{2}{7}$ . The value  $p(1) = \frac{2}{5}$  is also found in Milz and Strunz [7, eq. (22)], where they employed a quite different, interesting analytical framework, in which the principal variable of interest is the radial location in the Bloch ball of the reduced density matrix.

Further, we find  $\Pr \{ \det \xi^{PT} \geq 0 \}$  when the measure is multiplied by  $(\det \xi)^k$  for some fixed  $k \geq 0$  and  $\alpha = 1, 2, 3, \dots$ . For example when  $\alpha = 1$ ,  $\Pr \{ \det \xi^{PT} \geq 0 \} = 1 - \frac{2\Gamma(2k+4)^2}{\Gamma(k+2)\Gamma(3k+6)}$ . For  $\alpha = 2, 3, \dots$  we find that  $\Pr \{ \det \xi^{PT} \leq 0 \}$  is a product of a ratio of gamma functions with a polynomial in  $k$  with positive coefficients of degree  $2\alpha - 3$ . This combination is similar to our results for the full  $4 \times 4$  density matrices [16].

Section 2 contains the construction of the coordinate system used to set up the relevant definite integrals as well as the expression of the normalized measure in this system, and explains the relation of the values  $\alpha = \frac{1}{2}, 1, 2$  to real, complex, and quaternionic matrices.

In Section 3 the computation of  $\Pr \{ \det \xi^{PT} \geq 0 \}$  for any  $\alpha > 0$  is carried out. The computation starts with a five-fold iterated integral which is reduced to an integral of hypergeometric type and finally to a classical hypergeometric summation formula.

The measure of  $(\det \xi)^k$  type is studied in Section 4. The calculation of  $\Pr \{ \det \xi^{PT} \leq 0 \}$  is carried out only for integer values of  $\alpha$  for reasons of technical difficulty. As will be seen, even this integer case is quite complicated. Necessary integral formulas are derived in Section V.

## II. THE COORDINATE SYSTEM AND THE MEASURES

We construct a family of probability measures on  $\mathcal{X}$ , with a parameter  $\alpha$ , which agree with the normalized measures induced by the Hilbert-Schmidt measures on  $M_4(\mathbb{R}), M_4(\mathbb{C}), M_4(\mathbb{H})$  for  $\alpha = \frac{1}{2}, 1, 2$  respectively ( $\mathbb{H}$  denotes the quaternions). As in our previous studies [1, 16, 18], we use the Cholesky decomposition to define the measures. For  $x \in \mathbb{R}_{\geq 0}^4 \times \mathbb{C}^2$  let

$$C = \begin{bmatrix} x_1 & 0 & 0 & x_5 \\ 0 & x_2 & x_6 & 0 \\ 0 & 0 & x_3 & 0 \\ 0 & 0 & 0 & x_4 \end{bmatrix},$$

$$\xi = C^* C = \begin{bmatrix} x_1^2 & 0 & 0 & x_1 x_5 \\ 0 & x_2^2 & x_2 x_6 & 0 \\ 0 & x_2 \overline{x_6} & x_3^2 + |x_6|^2 & 0 \\ x_1 \overline{x_5} & 0 & 0 & x_4^2 + |x_5|^2 \end{bmatrix},$$

eventually we will impose the restriction  $\sum_{j=1}^4 x_j^2 + |x_5|^2 + |x_6|^2 = 1$  so that  $\text{tr} C = 1$ , but first we work with arbitrary positive-definite matrices.

To motivate the definition of the measures, we describe a simple model for the  $2 \times 2$  block. Consider the map defined on the subset  $H := \mathbb{R}_+^2 \times \mathbb{R}^m$  of  $\mathbb{R}^{2+m}$  (for some fixed

$m = 1, 2, \dots)$

$$\phi : (x_1, x_2, y_1, \dots, y_m) \mapsto (x_1^2, x_2^2 + |y|^2, x_1 y_1, \dots, x_1 y_m);$$

The Euclidean measure on  $H$  can be expressed as  $t_1^{-1/2} t_2^{-1/2} t_3^{m/2-1} dt_1 dt_2 dt_3 d\omega(y')$  where  $t_1 = x_1^2, t_2 = x_2^2$  and  $t_3 = |y|^2, y = |y| y'$  and  $d\omega(y')$  is the surface measure on the unit sphere  $\{y' \in \mathbb{R}^m : |y'|^2 = 1\}$ . The point  $(t_1, t_2, t_3) \in \mathbb{R}_+^3$ . The Jacobian of  $\phi$  equals  $4x_1^{1+m} x_2$ . The image of the measure on  $H$  under  $\phi$  is (constants are discarded)

$$t_1^{m/2} t_3^{m/2-1} dt_1 dt_2 dt_3 d\omega(y').$$

Now adjoin another copy of  $H$  and the map (a direct sum) and relabel to arrive at

$$\phi : (x_1, x_2, x_3, x_4, y^{(5)}, y^{(6)}) \in \mathbb{R}_+^4 \times \mathbb{R}^{2m} \mapsto (x_1^2, x_2^2, x_3^2 + |y^{(6)}|^2, x_4^2 + |y^{(5)}|^2, x_1 y^{(5)}, x_2 y^{(6)}),$$

and the measure

$$t_1^{m/2} t_2^{m/2} t_5^{m/2-1} t_6^{m/2-1} dt_1 dt_2 dt_3 dt_4 dt_5 dt_6 d\omega(y^{(5)'}) d\omega(y^{(6)'}).$$

In the cases  $m = 1, 2, 4$  this construction can be interpreted in terms of the Cholesky decomposition of a  $4 \times 4$  positive-definite X-matrix over  $\mathbb{R}, \mathbb{C}, \mathbb{H}$  respectively. In this situation  $\det \xi^{PT} = (t_1 t_4 + t_1 t_5 - t_2 t_6)(t_2 t_3 + t_2 t_6 - t_1 t_5)$  and the  $d\omega$  factor does not enter into the calculation, and so is replaced by 1. The same result is obtained if  $\xi_{14}, \xi_{23}$  are replaced by  $(t_1 t_5)^{1/2} e^{i\theta_5}, (t_2 t_6)^{1/2} e^{i\theta_6}$  respectively (with  $-\pi < \theta_5, \theta_6 \leq \pi$ ) and  $d\omega(y^{(5)'}) d\omega(y^{(6)'})$  is replaced by  $(\frac{1}{2\pi})^2 d\theta_5 d\theta_6$ . To sum up this discussion, the generic  $4 \times 4$  positive-definite complex X-matrix is

$$\begin{bmatrix} t_1 & 0 & 0 & (t_1 t_5)^{1/2} e^{i\theta_5} \\ 0 & t_2 & (t_2 t_6)^{1/2} e^{i\theta_6} & 0 \\ 0 & (t_2 t_6)^{1/2} e^{-i\theta_6} & t_3 + t_6 & 0 \\ (t_1 t_5)^{1/2} e^{-i\theta_5} & 0 & 0 & t_4 + t_5 \end{bmatrix}$$

and the parametrized measure is

$$t_1^\alpha t_2^\alpha t_5^{\alpha-1} t_6^{\alpha-1} dt_1 dt_2 dt_3 dt_4 dt_5 dt_6 d\theta_5 d\theta_6;$$

which has geometric interpretations when  $\alpha = \frac{m}{2}$ , with  $m = 1, 2, 4$ . The last step is to induce this measure on  $\{\xi : Tr \xi = 1\}$ , that is, on the unit simplex  $T_5$  in  $\mathbb{R}^5$  ( $t_2 = 1 - t_1 - \sum_{j=3}^5 t_j$ )

and drop  $dt_2$  from the measure. Also since we are concerned with only  $\det \xi^{PT}$  and  $\det \xi$  we also drop  $d\theta_5 d\theta_6$ .

We have arrived at the measure on  $T_5$

$$d\mu_\alpha = t_1^\alpha t_2^\alpha t_5^{\alpha-1} t_6^{\alpha-1} dt_1 dt_3 dt_4 dt_5 dt_6,$$

with normalization constant (a Dirichlet integral)

$$c_\alpha = \frac{\Gamma(4\alpha + 4)}{\Gamma(\alpha + 1)^2 \Gamma(\alpha)^2},$$

$$c_\alpha \int_{T^5} d\mu_\alpha = 1.$$

With these coordinates

$$\det \xi = t_1 t_2 t_3 t_4,$$

$$\det \xi^{PT} = (t_1 t_4 + t_1 t_5 - t_2 t_6) (t_2 t_3 + t_2 t_6 - t_1 t_5).$$

We introduce the desired coordinate system in two steps. The first step is:

$$\xi_{11} = t_1 = \frac{1}{2} (1 - s_1 + s_2), \xi_{22} = t_2 = \frac{1}{2} (s_1 + s_3),$$

$$\xi_{33} = t_3 + t_6 = \frac{1}{2} (s_1 - s_3), \xi_{44} = t_4 + t_5 = \frac{1}{2} (1 - s_1 - s_2),$$

$$t_5 = \frac{1}{2} s_4 (1 - s_1 - s_2), t_6 = \frac{1}{2} s_5 (s_1 - s_3),$$

$$t_3 = \frac{1}{2} (1 - s_5) (s_1 - s_3), t_4 = \frac{1}{2} (1 - s_4) (1 - s_1 - s_2),$$

where  $0 \leq s_1, s_4, s_5 \leq 1$  and  $|s_2| \leq 1 - s_1, |s_3| \leq s_1$ . The Jacobian (omitting  $t_2$  from the list  $(t)$ ) is

$$\frac{\partial(t)}{\partial(s)} = \frac{1}{16} (s_1 - s_3) (1 - s_1 - s_2),$$

and the measure and  $\det \xi^{PT}$  transform to

$$d\mu_\alpha = 2^{-4\alpha-2} ((1 - s_1)^2 - s_2^2)^\alpha (s_1^2 - s_3^2)^\alpha s_4^{\alpha-1} s_5^{\alpha-1} ds_1 ds_2 ds_3 ds_4 ds_5,$$

$$\det \xi^{PT} = \frac{1}{16} (((1 - s_1)^2 - s_2^2) - s_5 (s_1^2 - s_3^2)) ((s_1^2 - s_3^2) - s_4 ((1 - s_1)^2 - s_2^2)).$$

Since  $\det \xi^{PT}$  is even in  $s_2$  and  $s_3$  we can restrict to  $0 \leq s_2 \leq 1 - s_1, 0 \leq s_3 \leq s_1$  (a “quarter”

of  $\mathcal{X}$ , denoted by  $\mathcal{X}_0$ ) and multiply the measure by 4. The second step is to change variables

$$\begin{aligned}
s_2 &= \sqrt{(1-s_1)^2 - 4\delta_1}, s_3 = \sqrt{s_1^2 - 4\delta_2}, \\
\frac{\partial(s_2, s_3)}{\partial(\delta_1, \delta_2)} &= \frac{4}{\sqrt{(1-s_1)^2 - 4\delta_1} \sqrt{s_1^2 - 4\delta_2}}, \\
\det \xi^{PT} &= (\delta_1 - s_5\delta_2)(\delta_2 - s_4\delta_1), \\
\det \xi &= \delta_1\delta_2(1-s_4)(1-s_5), \\
\det \xi^{PT} - \det \xi &= (\delta_1 - \delta_2)(s_5\delta_2 - s_4\delta_1).
\end{aligned} \tag{1}$$

The measure transforms to

$$\begin{aligned}
d\nu_\alpha &= \frac{\delta_1^\alpha \delta_2^\alpha s_4^{\alpha-1} s_5^{\alpha-1}}{\sqrt{\frac{1}{4}(1-s_1)^2 - \delta_1} \sqrt{\frac{1}{4}s_1^2 - \delta_2}} ds_1 d\delta_1 d\delta_2 ds_4 ds_5, \\
0 \leq s_1, s_4, s_5 \leq 1, \quad 0 \leq \delta_1 &\leq \left(\frac{1-s_1}{2}\right)^2, \quad 0 \leq \delta_2 \leq \left(\frac{s_1}{2}\right)^2;
\end{aligned}$$

There is a beta-integral which we will use later, and also to verify the normalization (recall

$$B(a, b) := \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)} = \int_0^1 v^{a-1} (1-v)^{b-1} dv$$

$$\begin{aligned}
\int_0^c \frac{u^\alpha}{\sqrt{c-u}} du &= c^{\alpha+1/2} B\left(\alpha+1, \frac{1}{2}\right) \\
\int_{\mathcal{X}_0} d\nu_\alpha &= \frac{2^{-2-4\alpha}}{\alpha^2} B\left(\alpha+1, \frac{1}{2}\right)^2 \int_0^1 (1-s_1)^{2\alpha+1} s_1^{2\alpha+1} ds_1 \\
&= \frac{2^{-2-4\alpha}}{\alpha^2} \frac{\Gamma(\alpha+1)^2 \pi \Gamma(2\alpha+2)^2}{\Gamma(\alpha+\frac{3}{2})^2 \Gamma(4\alpha+4)} = \frac{1}{c_\alpha},
\end{aligned} \tag{3}$$

by use of the  $\Gamma$ -duplication formula  $\Gamma(2u) = \frac{1}{\sqrt{\pi}} 2^{2u-1} \Gamma(u) \Gamma(u+\frac{1}{2})$ . We will also use the Pochhammer symbol,  $(t)_0 = 1, (t)_{n+1} = (t)_n (t+n)$  for  $t \in \mathbb{C}$ .

We finish this section by describing the extreme values of  $\det \xi$ ,  $\det \xi^{PT}$  and  $\det \xi^{PT} - \det \xi$ . The maximum value of both  $\det \xi$  and  $\det \xi^{PT}$  is  $\frac{1}{256}$  for  $\xi = \frac{1}{4}I$  (identity matrix). The minimum value of both  $\det \xi^{PT}$  and  $\det \xi^{PT} - \det \xi$  is  $-\frac{1}{16}$  for  $s_1 = s_5 = 0, s_4 = 1, \delta_1 = \frac{1}{4}, \delta_2 = 0$  (and other matrices). To maximize  $\det \xi^{PT} - \det \xi = (\delta_1 - \delta_2)(s_5\delta_2 - s_4\delta_1)$  set  $s_5 = 1, s_4 = 0, \delta_1 = \left(\frac{1-s_1}{2}\right)^2, \delta_2 = \left(\frac{s_1}{2}\right)^2$  to obtain  $\frac{1}{16}s_1^2(1-2s_1)$  with maximum value  $\frac{1}{432}$  at  $s_1 = \frac{1}{3}$ . These extreme X-state values are identical to those for the full matrices.

### III. THE COMPUTATION OF $\Pr \{\det \xi^{PT} \geq 0\}$

The desired probability is the  $\nu_\alpha$ -measure of the set  $\{(s_1, \delta_1, \delta_2, s_4, s_5) : (\delta_1 - s_5\delta_2)(\delta_2 - s_4\delta_1) \geq 0\}$ , in other words, the definite integral of  $d\nu_\alpha$  over this set. We start the iterated integral with the variables  $s_4, s_5$ . There are apparently two possibilities for  $(\delta_1 - s_5\delta_2)(\delta_2 - s_4\delta_1) \geq 0$ :

- $\delta_1 - s_5\delta_2 \leq 0$  and  $\delta_2 - s_4\delta_1 \leq 0$ ; this implies  $\frac{\delta_1}{\delta_2} \leq s_5$  and  $\frac{\delta_2}{\delta_1} \leq s_4$ , but  $\max\left(\frac{\delta_1}{\delta_2}, \frac{\delta_2}{\delta_1}\right) > 1$  and one of the inequalities contradicts  $s_4, s_5 \leq 1$ , except for the trivial case  $\delta_1 = \delta_2, s_3 = 1 = s_4$ , included in the following case (the products of the two pairs of eigenvalues of  $\xi^{PT}$  are  $(\delta_1 - s_5\delta_2)$  and  $(\delta_2 - s_4\delta_1)$ , so this demonstrates that  $\xi^{PT}$  can have at most one negative eigenvalue);
- $\delta_1 - s_5\delta_2 \geq 0$  and  $\delta_2 - s_4\delta_1 \geq 0$ ; equivalent to  $\frac{\delta_1}{\delta_2} \geq s_5$  and  $\frac{\delta_2}{\delta_1} \geq s_4$ . Thus  $\delta_2 \leq \delta_1$  imposes the bounds  $0 \leq s_4 \leq \frac{\delta_2}{\delta_1} \leq 1$  and  $0 \leq s_5 \leq 1 \leq \frac{\delta_1}{\delta_2}$ . Similarly  $\delta_1 \leq \delta_2$  imposes the bounds  $0 \leq s_4 \leq 1$  and  $0 \leq s_5 \leq \frac{\delta_1}{\delta_2} \leq 1$ . In both cases the integral of  $s_4^{\alpha-1}s_5^{\alpha-1}ds_4ds_5$  over this region equals

$$\frac{1}{\alpha^2} \left( \min \left( \frac{\delta_2}{\delta_1}, \frac{\delta_1}{\delta_2} \right) \right)^\alpha.$$

As a side observation, the computation of  $\Pr \{\det \xi^{PT} \geq \det \xi\} = \Pr \{(\delta_1 - \delta_2)(s_5\delta_2 - s_4\delta_1) \geq 0\}$  starts with integrating  $s_4^{\alpha-1}s_5^{\alpha-1}ds_4ds_5$  over the region  $\delta_1 \geq \delta_2, 0 \leq s_4 \leq \frac{\delta_2}{\delta_1}s_5$ , or the region  $\delta_2 \geq \delta_1, 0 \leq s_5 \leq \frac{\delta_1}{\delta_2}s_4$ ; the result in both cases is  $\frac{1}{2\alpha^2} \left( \min \left( \frac{\delta_2}{\delta_1}, \frac{\delta_1}{\delta_2} \right) \right)^\alpha$ . Since the rest of the probability calculation is the same for both, we see that  $\Pr \{\det \xi^{PT} \geq \det \xi\} = \frac{1}{2} \Pr \{\det \xi^{PT} > 0\}$ , analogously to the general  $4 \times 4$  situation, as we discussed in earlier work [18].

By symmetry, it suffices to integrate over  $\{0 \leq s_1 \leq \frac{1}{2}\}$  and double the result. Denote  $a := \left(\frac{1-s_1}{2}\right)^2$  and  $b := \left(\frac{s_1}{2}\right)^2$ , thus  $0 \leq b \leq a \leq \frac{1}{4}$ . In the iterated triple integral first integrate with respect to  $\delta_1$ . Let

$$\begin{aligned} I_\alpha &:= \frac{2}{\alpha^2} \int_0^{1/2} ds_1 \int_0^b \frac{\delta_2^\alpha}{\sqrt{b-\delta_2}} d\delta_2 \left\{ \int_0^{\delta_2} \left( \frac{\delta_1}{\delta_2} \right)^\alpha \frac{\delta_1^\alpha}{\sqrt{a-\delta_1}} d\delta_1 + \int_{\delta_2}^a \left( \frac{\delta_2}{\delta_1} \right)^\alpha \frac{\delta_1^\alpha}{\sqrt{a-\delta_1}} d\delta_1 \right\} \\ &= \frac{2}{\alpha^2} \int_0^{1/2} ds_1 \int_0^b \frac{d\delta_2}{\sqrt{b-\delta_2}} \left\{ \int_0^{\delta_2} \frac{\delta_1^{2\alpha}}{\sqrt{a-\delta_1}} d\delta_1 + \delta_2^{2\alpha} \int_{\delta_2}^a \frac{d\delta_1}{\sqrt{a-\delta_1}} \right\}. \end{aligned}$$



In the  $\{\cdot\}$  expression, the second integral equals  $2\sqrt{a-\delta_2}$ ; for the first one, interchange the order of integration (over  $0 \leq \delta_1 \leq \delta_2 \leq b$ ) to obtain

$$\int_0^b \frac{\delta_1^{2\alpha}}{\sqrt{a-\delta_1}} d\delta_1 \int_{\delta_1}^b \frac{d\delta_2}{\sqrt{b-\delta_2}} = 2 \int_0^b \delta_1^{2\alpha} \sqrt{\frac{b-\delta_1}{a-\delta_1}} d\delta_1.$$

Thus,

$$I_\alpha = \frac{4}{\alpha^2} \int_0^{1/2} ds_1 \int_0^b v^{2\alpha} \left\{ \sqrt{\frac{b-v}{a-v}} + \sqrt{\frac{a-v}{b-v}} \right\} dv.$$

This integral can be directly evaluated for any  $\alpha$  with  $2\alpha \in \mathbb{Z}_+$  with elementary methods. However, this integral is one of a parametrized family which all have closed forms for their values. The integrals are denoted by

$$I(m, n) := \int_0^{\frac{1}{2}} ds \int_0^b v^m \left\{ (a-v)^n \sqrt{\frac{a-v}{b-v}} + (b-v)^n \sqrt{\frac{b-v}{a-v}} \right\} dv.$$

The formulas for  $(m, n) = (2\alpha, 0)$  for  $\alpha > 0$  and for  $m, n = 0, 1, 2, 3, \dots$  are derived in Section V.

From Proposition V.2 it follows that

$$I_\alpha = \frac{4}{\alpha^2} I(2\alpha, 0) = \frac{\pi}{2^{2+8\alpha}} \frac{\Gamma(2\alpha)\Gamma(2\alpha)}{\Gamma(2\alpha + \frac{3}{2}) \Gamma(2\alpha + \frac{5}{2})}.$$

When  $2\alpha \in \mathbb{Z}_+$  the reciprocal of  $I_\alpha$  is an integer. In fact,

$$I_\alpha^{-1} = 2(4\alpha + 3) \binom{2\alpha + 2}{2}^2 \binom{4\alpha + 1}{2\alpha + 2}^2.$$

Finally, we obtain

$$\begin{aligned} \Pr \{ \det \xi^{PT} \geq 0 \} &= c_\alpha I_\alpha = \frac{\pi}{2^{2+8\alpha}} \frac{\Gamma(4\alpha + 4) \Gamma(2\alpha) \Gamma(2\alpha)}{\Gamma(\alpha + 1)^2 \Gamma(\alpha)^2 \Gamma(2\alpha + \frac{3}{2}) \Gamma(2\alpha + \frac{5}{2})} \\ &= \frac{1}{\sqrt{2\pi}} \frac{\Gamma(\alpha + \frac{1}{2})^2 \Gamma(\alpha + \frac{3}{2})}{\Gamma(\alpha + \frac{3}{4}) \Gamma(\alpha + 1) \Gamma(\alpha + \frac{5}{4})} =: p(\alpha) \end{aligned} \quad (4)$$

by repeated use of the  $\Gamma$ -duplication formula. If  $\alpha = m$  is an integer, then  $c_\alpha = \frac{(m-1)^2 (4m+3)!}{m!^4}$  and  $p(\alpha)$  is rational. If  $\alpha + \frac{1}{2} = m$ , then  $c_\alpha = \frac{4(m - \frac{1}{2})^2 (4m+2)!}{\pi^2 (\frac{1}{2})_m}$

and  $p(\alpha) \pi^2$  is rational. The asymptotic formula  $\frac{\Gamma(u+a)}{\Gamma(u+b)} \sim u^{a-b}$  as  $u \rightarrow \infty$  shows that

$p(\alpha) \sim \frac{1}{\sqrt{2\pi\alpha}}$  as  $\alpha \rightarrow \infty$ . For example,  $p(10) = 0.12683\dots$  and  $\frac{1}{\sqrt{20\pi}} = 0.12616\dots$

### A. Minimally degenerate matrices

In our previous work [18], we considered the separability probability of a minimally degenerate density matrix, and found numerical and formulaic evidence that this probability is exactly one half of the unrestricted one. We can prove this relation in the present X-matrix case. From  $\det \xi = \delta_1 \delta_2 (1 - s_4) (1 - s_5)$ , we see that a necessary condition for minimal degeneracy is that one of  $\delta_1, \delta_2, (1 - s_4), (1 - s_5)$  vanishes. The possibility  $\delta_1 = 0$  or  $\delta_2 = 0$  is not minimal, for suppose  $\delta_1 = 0$  then (see (1))  $s_2 = 1 - s_1$  which implies  $t_4 = 0 = t_5$ , reducing the dimension by two. This leaves the cases  $s_4 = 1$  or  $s_5 = 1$  (for example,  $s_5 = 1$  is equivalent to  $\xi_{22}\xi_{33} - |\xi_{23}|^2 = 0$ ) which remove only one dimension (degree of freedom). So the minimally degenerate subset of  $\mathcal{X}$  consists of two almost (i.e. the intersection has measure zero) disjoint subsets, one with  $s_4 = 1$  and one with  $s_5 = 1$ . It suffices to compute the probability for one of these, say  $s_5 = 1$ . First we compute the normalizing constant: the calculation is the same as in (3) except for the factor  $\frac{1}{\alpha}$  from  $\int_0^1 s_5^{\alpha-1} ds_5$ , thus the constant is  $\frac{c\alpha}{\alpha}$ . We see  $\det \xi^{PT} = (\delta_1 - \delta_2) (\delta_2 - s_4 \delta_1) \geq 0$  if  $\delta_1 \geq \delta_2$  and  $0 \leq s_4 \leq \frac{\delta_2}{\delta_1}$ , or  $\delta_1 < \delta_2$  and  $s_4 \geq \frac{\delta_2}{\delta_1} > 1$ ; as before the second case is impossible. Thus the first step of integration (for  $s_4$ ) yields  $\frac{1}{\alpha} \left( \frac{\delta_2}{\delta_1} \right)^\alpha$  for  $\delta_1 \geq \delta_2$  and zero otherwise. In contrast to the earlier computation, there is no  $s_1 \leftrightarrow 1 - s_1$  symmetry so  $0 \leq s_1 \leq \frac{1}{2}$  and  $\frac{1}{2} \leq s_1 \leq 1$  are handled separately.

If  $0 \leq s_1 \leq \frac{1}{2}$  (so that  $b = \left(\frac{s_1}{2}\right)^2 \leq \left(\frac{1-s_1}{2}\right)^2 = a$ ), then the remaining triple integral is

$$\begin{aligned} & \frac{1}{\alpha} \int_0^{1/2} ds_1 \int_0^b \frac{\delta_2^\alpha}{\sqrt{b - \delta_2}} d\delta_2 \int_{\delta_2}^a \left( \frac{\delta_2}{\delta_1} \right)^\alpha \frac{\delta_1^\alpha}{\sqrt{a - \delta_1}} d\delta_1 \\ &= \frac{2}{\alpha} \int_0^{1/2} ds_1 \int_0^b \delta_2^{2\alpha} \sqrt{\frac{a - \delta_2}{b - \delta_2}} d\delta_2. \end{aligned}$$

If  $\frac{1}{2} \leq s_1 \leq 1$  (so that  $b \geq a \geq \delta_1 \geq \delta_2$ ), then the remaining triple integral is

$$\begin{aligned} & \frac{1}{\alpha} \int_{1/2}^1 ds_1 \int_0^a \frac{\delta_2^\alpha}{\sqrt{b - \delta_2}} d\delta_2 \int_{\delta_2}^a \left( \frac{\delta_2}{\delta_1} \right)^\alpha \frac{\delta_1^\alpha}{\sqrt{a - \delta_1}} d\delta_1 \\ &= \frac{2}{\alpha} \int_{1/2}^1 ds_1 \int_0^a \delta_2^{2\alpha} \sqrt{\frac{a - \delta_2}{b - \delta_2}} d\delta_2. \end{aligned}$$

In the latter expression change variables  $s = 1 - s_1$  which interchanges  $a$  and  $b$  with the result

$$\frac{2}{\alpha} \int_0^{1/2} ds \int_0^b \delta_2^{2\alpha} \sqrt{\frac{b - \delta_2}{a - \delta_2}} d\delta_2$$

and adding the two parts leads to

$$\frac{2}{\alpha} \int_0^{1/2} ds \int_0^b \delta_2^{2\alpha} \left\{ \sqrt{\frac{b-\delta_2}{a-\delta_2}} + \sqrt{\frac{a-\delta_2}{b-\delta_2}} \right\} d\delta_2 = \frac{2}{\alpha} I(2\alpha, 0).$$

Thus

$$\Pr \{ \det \xi^{PT} \geq 0 \} = \frac{c_\alpha}{\alpha} \frac{2}{\alpha} I(2\alpha, 0) = \frac{1}{2} p(\alpha),$$

see equation (4).

#### IV. THE MEASURE $(\det \xi)^k d\nu_\alpha$

Here we compute  $\Pr \{ \det \xi^{PT} < 0 \}$  when  $\mathcal{X}$  is furnished with the normalization of the measure  $(\det \xi)^k d\nu_\alpha$ , for  $\alpha, k \in \mathbb{Z}_+$ . It appears possible to carry out the calculations for fixed integers  $k$  and arbitrary  $\alpha > 0$ , but with the goal of allowing  $k$  as a free parameter, technical factors impel us to restrict to integer  $\alpha$ . Recall  $\det \xi = \delta_1 \delta_2 (1 - s_4) (1 - s_5)$ . The normalization constant is

$$c_{\alpha,k} = \frac{\Gamma(4\alpha + 4k + 4)}{\Gamma(k + \alpha + 1)^2 \Gamma(k + 1)^2 \Gamma(\alpha)^2},$$

and the measure is

$$\frac{\delta_1^{\alpha+k} \delta_2^{\alpha+k} s_4^{\alpha-1} s_5^{\alpha-1} (1 - s_4)^k (1 - s_5)^k}{\sqrt{\frac{1}{4} (1 - s_1)^2 - \delta_1} \sqrt{\frac{1}{4} s_1^2 - \delta_2}} ds_1 d\delta_1 d\delta_2 ds_4 ds_5.$$

Some experimenting suggests that it is more tractable to compute  $\Pr \{ \det \xi^{PT} < 0 \}$ . Then, the first step is to compute (with  $\delta_0 = \min \left( \frac{\delta_1}{\delta_2}, \frac{\delta_2}{\delta_1} \right)$ )

$$\int_0^1 u^{\alpha-1} (1 - u)^k du \int_{\delta_0}^1 v^{\alpha-1} (1 - v)^k dv = \frac{\Gamma(\alpha) \Gamma(k + 1)}{\Gamma(\alpha + k + 1)} \int_{\delta_0}^1 v^{\alpha-1} (1 - v)^k dv,$$

where  $\{u, v\} = \{s_4, s_5\}$  (depending on whether  $\delta_1 \geq \delta_2$ ). The second integral is an incomplete Beta integral. As discussed above, the restriction  $\alpha \in \mathbb{Z}_+$  leads to a feasible calculation. We use this simple antiderivative formula:

$$\begin{aligned} \frac{d}{dv} \sum_{j=0}^{\alpha-1} (-1)^{j+1} \frac{(1-\alpha)_j}{(k+1)_{j+1}} v^{\alpha-1-j} (1-v)^{k+j+1} &= v^{\alpha-1} (1-v)^k, \\ \int_{\delta_0}^1 v^{\alpha-1} (1-v)^k dv &= \sum_{j=0}^{\alpha-1} (-1)^j \frac{(1-\alpha)_j}{(k+1)_{j+1}} \delta_0^{\alpha-1-j} (1-\delta_0)^{k+j+1}. \end{aligned} \quad (5)$$

From this point on, we work with each term in the sum separately, in the triple integrals that remain to be evaluated. At the end, the parts will be summed over  $j$  to get the desired probability.

If  $\delta_1 \leq \delta_2$  then  $\delta_1^{\alpha+k} \delta_2^{\alpha+k} \delta_0^{\alpha-1-j} (1-\delta_0)^{k+j+1} = \delta_1^{2\alpha+k-1-j} (\delta_2 - \delta_1)^{k+j+1}$ , otherwise  $\delta_1^{\alpha+k} \delta_2^{\alpha+k} \delta_0^{\alpha-1-j} (1-\delta_0)^{k+j+1} = \delta_2^{2\alpha+k-1-j} (\delta_1 - \delta_2)^{k+j+1}$ . As in the previous section, we restrict to  $0 \leq s_1 \leq \frac{1}{2}$  and set  $a = \frac{(1-s_1)^2}{4}$ ,  $b = \frac{s_1^2}{4}$ .

The typical term  $\delta_1^{\alpha+k} \delta_2^{\alpha+k} \delta_0^{\alpha-1-j} (1-\delta_0)^{k+j+1}$  produces the integral

$$\begin{aligned}
& \int_0^{\frac{1}{2}} ds_1 \int_0^b \frac{d\delta_2}{\sqrt{b-\delta_2}} \\
& \times \left\{ \int_0^{\delta_2} \frac{\delta_1^{2\alpha+k-1-j} (\delta_2 - \delta_1)^{k+j+1}}{\sqrt{a-\delta_1}} d\delta_1 + \delta_2^{2\alpha+k-1-j} \int_{\delta_2}^a \frac{(\delta_1 - \delta_2)^{k+j+1}}{\sqrt{a-\delta_1}} d\delta_1 \right\} \\
& = \int_0^{\frac{1}{2}} ds_1 \int_0^b \frac{\delta_1^{2\alpha+k-1-j} d\delta_1}{\sqrt{a-\delta_1}} \int_{\delta_1}^b \frac{(\delta_2 - \delta_1)^{k+j+1} d\delta_2}{\sqrt{b-\delta_2}} \\
& + \int_0^{\frac{1}{2}} ds_1 \int_0^b \frac{\delta_2^{2\alpha+k-1-j} d\delta_2}{\sqrt{b-\delta_2}} \int_{\delta_2}^a \frac{(\delta_1 - \delta_2)^{k+j+1}}{\sqrt{a-\delta_1}} d\delta_1 \\
& = B \left( k+j+2, \frac{1}{2} \right) \int_0^{\frac{1}{2}} ds_1 \\
& \times \left\{ \int_0^b (b-\delta_1)^{k+j+3/2} \frac{\delta_1^{2\alpha+k-1-j} d\delta_1}{\sqrt{a-\delta_1}} + \int_0^b (a-\delta_2)^{k+j+3/2} \frac{\delta_2^{2\alpha+k-1-j} d\delta_2}{\sqrt{b-\delta_2}} \right\} \\
& = \frac{(k+j+1)!}{\left(\frac{1}{2}\right)_{k+j+2}} \int_0^{\frac{1}{2}} ds_1 \\
& \times \int_0^b v^{2\alpha+k-1-j} \left\{ (b-v)^{k+j+1} \sqrt{\frac{b-v}{a-v}} + (a-v)^{k+j+1} \sqrt{\frac{a-v}{b-v}} \right\} dv \\
& = \frac{(k+j+1)!}{\left(\frac{1}{2}\right)_{k+j+2}} I(2\alpha+k-1-j, k+j+1).
\end{aligned}$$

(Note  $B(m+1, \frac{1}{2}) = \frac{m!}{\left(\frac{1}{2}\right)_{m+1}}$ .) The proof and statement of the  $I(m, n)$  formula are in Prop.V.1. Then

$$\begin{aligned}
\Pr \{ \det \xi^{PT} \leq 0 \} &= 2c_{\alpha,k} B(\alpha, k+1) \\
&\times \sum_{j=0}^{\alpha-1} (-1)^j \frac{(1-\alpha)_j (k+j+1)!}{(k+1)_{j+1} \left(\frac{1}{2}\right)_{k+j+2}} I(2\alpha+k-1-j, k+j+1).
\end{aligned}$$

By formula (V.1)

$$I(2\alpha+k-1-j, k+j+1) = \frac{(2\alpha+k-1-j)!^2 (2\alpha+2k+1)! \left(\frac{5}{2}\right)_{k+j}}{2^{4\alpha+4k+3} (4\alpha+3k-j+1)! \left(\frac{5}{2}\right)_{2\alpha+2k}}.$$

We combine the various terms to arrive at:

$$\begin{aligned}
\Pr \{ \det \xi^{PT} \leq 0 \} &= \sum_{j=0}^{\alpha-1} \frac{2\Gamma(2\alpha+2k+2)^2 \Gamma(2\alpha+k-j)^2}{\Gamma(\alpha+k+1)^3 \Gamma(\alpha-j) \Gamma(4\alpha+3k-j+2)} \\
&= \frac{\Gamma(2\alpha+2k+3)^2}{2\Gamma(\alpha+k+2) \Gamma(4\alpha+3k+2)} \\
&\times \sum_{j=0}^{\alpha-1} \frac{(-1)^j}{(\alpha-1)! (\alpha+k+1)} (\alpha+k+1)_{\alpha-1-j}^2 (-1-3k-4\alpha)_j;
\end{aligned}$$

the  $j$ -sum is a polynomial of degree  $2\alpha-3-j$  in  $k$  (the factor  $(\alpha+k+1)$  obviously cancels when  $j \leq \alpha-2$ , and when  $j = \alpha-1$  the last factor equals  $-3(\alpha+k+1)(-1-3k-4\alpha)_{\alpha-2}$ ). This phenomenon is qualitatively similar to our results for the general  $4 \times 4$  situation. In particular for  $\alpha = 1$

$$\Pr \{ \det \xi^{PT} \leq 0 \} = \frac{2\Gamma(2k+4)^2}{\Gamma(k+2) \Gamma(3k+6)} = \frac{2^{4k+7} \left(\frac{1}{2}\right)_{k+2}^2}{3^{3k+5} \left(\frac{1}{3}\right)_{k+2} \left(\frac{2}{3}\right)_{k+2}},$$

and for  $\alpha = 2$

$$\Pr \{ \det \xi^{PT} \leq 0 \} = \frac{2(k+6)\Gamma(2k+6)^2}{3\Gamma(k+3)\Gamma(3k+9)}.$$

#### A. Probability of $\det \xi^{PT} \geq \det \xi$

Next we compute  $\Pr \{ \det \xi^{PT} \geq \det \xi \}$  for  $\alpha = 1$  and the measure  $(\det \xi)^k d\nu_\alpha$ . As above, it is neater to work with the complement. From equation (2),  $\det \xi^{PT} - \det \xi = (\delta_1 - \delta_2)(s_5\delta_2 - s_4\delta_1)$ . To make  $\det \xi^{PT} - \det \xi \leq 0$  either  $\delta_1 \geq \delta_2$  and  $s_4 \geq \frac{\delta_2}{\delta_1}s_5$  or  $\delta_1 < \delta_2$  and  $s_5 > \frac{\delta_1}{\delta_2}s_4$ . The first two integrations for  $\delta_1 \geq \delta_2$  are

$$\begin{aligned}
&(\delta_1\delta_2)^{k+1} \int_0^1 (1-s_5)^k ds_5 \int_{\frac{\delta_2}{\delta_1}s_5}^1 (1-s_4)^k ds_4 \\
&= \frac{(\delta_1\delta_2)^{k+1}}{k+1} \int_0^1 (1-s_5)^k \left(1 - \frac{\delta_2}{\delta_1}s_5\right)^{k+1} ds_5 \\
&= \frac{\delta_2^{k+1}}{k+1} \int_0^1 (1-s_5)^k (\delta_1 - \delta_2 + \delta_2(1-s_5))^{k+1} ds_5 \\
&= \frac{1}{k+1} \sum_{j=0}^{k+1} \binom{k+1}{j} (\delta_1 - \delta_2)^j \delta_2^{2k+2-j} \int_0^1 (1-s_5)^{2k+1-j} ds_5 \\
&= \frac{1}{k+1} \sum_{j=0}^{k+1} \binom{k+1}{j} \frac{(\delta_1 - \delta_2)^j \delta_2^{2k+2-j}}{2k+2-j};
\end{aligned}$$

similarly for  $\delta_1 < \delta_2$  the value of the integral is  $\frac{1}{k+1} \sum_{j=0}^{k+1} \binom{k+1}{j} \frac{(\delta_2 - \delta_1)^j \delta_1^{2k+2-j}}{2k+2-j}$ . Proceeding as before and with the same notations carry out the remaining integrations on the term with fixed  $j$ , for  $0 \leq j \leq k+1$ . Assume  $0 \leq s_1 \leq \frac{1}{2}$ , then we obtain

$$\begin{aligned}
& \int_0^{\frac{1}{2}} ds_1 \int_0^b \frac{d\delta_2}{\sqrt{b-\delta_2}} \left\{ \int_0^{\delta_2} \frac{\delta_1^{2k+2-j} (\delta_2 - \delta_1)^j}{\sqrt{a-\delta_1}} d\delta_1 + \delta_2^{2k+2-j} \int_{\delta_2}^a \frac{(\delta_1 - \delta_2)^j}{\sqrt{a-\delta_1}} d\delta_1 \right\} \\
&= \int_0^{\frac{1}{2}} ds_1 \int_0^b \frac{\delta_1^{2k+2-j} d\delta_1}{\sqrt{a-\delta_1}} \int_{\delta_1}^b \frac{(\delta_2 - \delta_1)^j d\delta_2}{\sqrt{b-\delta_2}} + \int_0^b \frac{\delta_2^{2k+2-j} d\delta_2}{\sqrt{b-\delta_2}} \int_{\delta_2}^a \frac{(\delta_1 - \delta_2)^j}{\sqrt{a-\delta_1}} d\delta_1 \\
&= B \left( j+1, \frac{1}{2} \right) \int_0^{\frac{1}{2}} ds_1 \left\{ \int_0^b (b-\delta_1)^{j+1/2} \frac{\delta_1^{2k+2-j} d\delta_1}{\sqrt{a-\delta_1}} + \int_0^b (a-\delta_2)^{j+1/2} \frac{\delta_2^{2k+2-j} d\delta_2}{\sqrt{b-\delta_2}} \right\} \\
&= \frac{j!}{\left(\frac{1}{2}\right)_{j+1}} \int_0^{\frac{1}{2}} ds_1 \int_0^b v^{2k+2-j} \left\{ (b-v)^j \sqrt{\frac{b-v}{a-v}} + (a-v)^j \sqrt{\frac{a-v}{b-v}} \right\} dv \\
&= \frac{j!}{\left(\frac{1}{2}\right)_{j+1}} I(2k+2-j, j).
\end{aligned}$$

Thus

$$\begin{aligned}
\Pr \{ \det \xi^{PT} \leq \det \xi \} &= 2c_{1,k} \sum_{j=0}^{k+1} \binom{k+1}{j} \frac{j!}{(k+1)(2k+2-j)\left(\frac{1}{2}\right)_{j+1}} I(2k+2-j, j) \\
&= 2^{2k-1} \frac{\left(\frac{3}{2}\right)_k^2 \left(\frac{5}{2}\right)_k}{(k+1)! \left(\frac{5}{2}\right)_{2k+1}} \sum_{j=0}^{k+1} \frac{(-k-1)_j (-4k-6)_j}{(-2k-2)_j (-2k-1)_j},
\end{aligned}$$

after simplification. The sum is a truncated  ${}_3F_2$  series.

With more technical details, we can determine  $\Pr \{ \det \xi^{PT} \leq \det \xi \}$  for the measure  $(\det \xi)^k d\nu_\alpha$  for  $\alpha, k = 1, 2, 3, \dots$ . Proceeding as for  $\alpha = 1$  we start with the integral

$$(\delta_1 \delta_2)^{\alpha+k} \int_0^1 s_5^{\alpha-1} (1-s_5)^k ds_5 \int_{s_5 \delta_0}^1 s_4^{\alpha-1} (1-s_4)^k ds_4,$$

where  $\delta_0 = \frac{\delta_2}{\delta_1}$  and  $0 \leq \delta_2 \leq \delta_1$ ; and there is a similar expression when  $\delta_1 \leq \delta_2$ . Use formula (5) (with  $\delta_0$  replaced by  $s_5 \delta_0$ ) to get the value

$$\begin{aligned}
& \delta_2^k \int_0^1 s_5^{\alpha-1} (1-s_5)^k \sum_{j=0}^{\alpha-1} (-1)^j \frac{(1-\alpha)_j}{(k+1)_{j+1}} \delta_2^{\alpha-1-j} s_5^{\alpha-1-j} (\delta_1 - \delta_2 + (1-s_5)\delta_2)^{k+j+1} ds_5 \\
&= \sum_{j=0}^{\alpha-1} (-1)^j \frac{(1-\alpha)_j}{(k+1)_{j+1}} \sum_{i=0}^{k+j+1} \binom{k+1+j}{i} B(2\alpha-j-1, 2k+j-i+2) (\delta_1 - \delta_2)^i \delta_2^{2k+2\alpha-i} \\
&= \sum_{i=0}^{k+\alpha} (\delta_1 - \delta_2)^i \delta_2^{2k+2\alpha-i} \sigma(k, \alpha, i),
\end{aligned}$$

where

$$\sigma(k, \alpha, i) = \sum_{j=\max(0, i-k-1)}^{\alpha-1} \frac{k! (\alpha-1)! (2\alpha-2-j)! (2k+j-i+1)!}{i! (\alpha-1-j)! (k+1+j-i)! (2k+2\alpha-i)!}.$$

For  $0 \leq i \leq k$

$$\sigma(k, \alpha, i) = \frac{k! (2k+1-i)! (2\alpha-2)!}{i! (k+1-i)! (2k+2\alpha-1)!} \sum_{j=0}^{\alpha-1} \frac{(1-\alpha)_j (2k+2-i)_j}{(2-2\alpha)_j (k+2-i)_j},$$

and for  $k+1 \leq i \leq k+\alpha$

$$\sigma(k, \alpha, i) = \left\{ \alpha \binom{k+\alpha}{\alpha} \right\}^{-2} \binom{k+\alpha}{i}.$$

Similarly, the integral equals  $\sum_{i=0}^{k+\alpha} (\delta_2 - \delta_1)^i \delta_1^{2k+2\alpha-i} \sigma(k, \alpha, i)$  when  $\delta_1 \leq \delta_2$ . With the same steps as above, we obtain

$$\Pr \{ \det \xi^{PT} \leq \det \xi \} = 2c_{\alpha, k} \sum_{i=0}^{k+\alpha} \sigma(k, \alpha, i) \frac{i!}{\left(\frac{1}{2}\right)_{i+1}} I(2k+2\alpha-i, i).$$

Some simplification may be possible.

## V. INTEGRAL FORMULAS

In this section we compute closed expressions for

$$I(m, n) := \int_0^{\frac{1}{2}} ds \int_0^b v^m \left\{ (a-v)^n \sqrt{\frac{a-v}{b-v}} + (b-v)^n \sqrt{\frac{b-v}{a-v}} \right\} dv,$$

for  $m, n = 0, 1, 2, 3, \dots$  and for  $(m, n) = (2\alpha, 0)$  with  $\alpha > 0$ ; where  $a = \left(\frac{1-s}{2}\right)^2$ ,  $b = \left(\frac{s}{2}\right)^2$  so that  $0 \leq b \leq a \leq \frac{1}{4}$ . The auxiliary formula

$$\begin{aligned} S(m, n) &:= \sum_{i=0}^m \frac{(-m)_i (n+1)_i}{i! (m+n+2)_i} \sum_{j=0}^n \frac{(-n)_j \left(\frac{1}{2}-n\right)_j}{j! \left(\frac{1}{2}\right)_j} \frac{1}{i+j+\frac{1}{2}} \\ &= 2^{2m+2n} \frac{m! (m+n)! (m+n+1)! \left(\frac{1}{2}\right)_n}{n! (n+2m+1)! \left(\frac{1}{2}\right)_{m+n+1}} \end{aligned}$$

is proved in [20, Prop. 2].

**Proposition V.1** For  $m, n = 0, 1, 2, 3, \dots$

$$\begin{aligned} I(m, n) &= \int_0^{\frac{1}{2}} ds \int_0^b v^m \left\{ (a-v)^n \sqrt{\frac{a-v}{b-v}} + (b-v)^n \sqrt{\frac{b-v}{a-v}} \right\} dv \\ &= 2^{-4m-4n-5} B(m+1, n+2) S(m, n+1) \\ &= 2^{-2m-2n-3} \frac{(m!)^2 (m+n+1)! \left(\frac{1}{2}\right)_{n+1}}{(2m+n+2)! \left(\frac{1}{2}\right)_{m+n+2}}. \end{aligned}$$

**Proof** Set  $z = 1 - 2s$ ,  $u^2 = \frac{b-v}{a-v}$ ,  $a = \frac{1}{16}(1+z)^2$ ,  $b = \frac{1}{16}(1-z)^2$  then

$$\begin{aligned} b - v &= \frac{u^2 z}{4(1-u^2)}, a - v = \frac{z}{4(1-u^2)}, \\ v &= \frac{(1-z)^2 - u^2(1+z)^2}{16(1-u^2)}, dv = -\frac{uz}{2(1-u^2)^2} du, \\ 0 \leq z \leq 1, 0 \leq u &\leq \frac{1-z}{1+z}. \end{aligned}$$

For changing the order of integration note that  $0 \leq z \leq 1$  and  $0 \leq u \leq \frac{1-z}{1+z}$  is equivalent to  $0 \leq u \leq 1$  and  $0 \leq z \leq \frac{1-u}{1+u}$ . Thus

$$\begin{aligned} &\left\{ (a-v)^n \sqrt{\frac{a-v}{b-v}} + (b-v)^n \sqrt{\frac{b-v}{a-v}} \right\} ds dv \\ &= - \left\{ \left( \frac{u^2 z}{4(1-u^2)} \right)^n u^2 + \left( \frac{z}{4(1-u^2)} \right)^n \right\} \frac{z dz du}{4(1-u^2)^2} \\ &= -2^{-2n-2} z^{n+1} \frac{u^{2n+2} + 1}{(1-u^2)^{n+2}} dz du. \end{aligned}$$

Then introduce the new variable  $y$ :

$$\begin{aligned} z &= \frac{1-u}{1+u} y, \frac{z^{n+1}}{(1-u^2)^{n+2}} dz = \frac{y^{n+1}}{(1+u)^{2n+4}} dy, \\ v &= \frac{1}{16} (1-y) \left( 1 - \left( \frac{1-u}{1+u} \right)^2 y \right), \\ 0 \leq u &\leq 1, 0 \leq y \leq 1, \end{aligned}$$

and the integral is transformed to

$$\begin{aligned} &2^{-4m-2n-2} \int_0^1 \frac{u^{2n+2} + 1}{(1+u)^{2n+4}} du \int_0^1 y^{n+1} (1-y)^m \left( 1 - \left( \frac{1-u}{1+u} \right)^2 y \right)^m dy \\ &= 2^{-4m-2n-2} B(m+1, n+2) \sum_{i=0}^m \frac{(-m)_i (n+2)_i}{i! (m+n+3)_i} \int_0^1 \frac{u^{2n+2} + 1}{(1+u)^{2n+4}} \left( \frac{1-u}{1+u} \right)^{2i} du, \end{aligned} \tag{6}$$

by use of the binomial expansion and

$$\int_0^1 y^{n+1} (1-y)^m y^i dy = B(m+1, n+2+i) = B(m+1, n+2) \frac{(n+2)_i}{(m+n+3)_i}.$$



Let  $w = \frac{1-u}{1+u}$ ,  $u = \frac{1-w}{1+w}$ , then  $du = -\frac{2}{(1+w)^2}dw$ ,  $\frac{1}{1+u} = \frac{1}{2}(1+w)$ , and

$$\begin{aligned} \int_0^1 \frac{u^{2n+2}+1}{(1+u)^{2n+4}} \left(\frac{1-u}{1+u}\right)^{2i} du &= 2^{-2n-3} \int_0^1 \left\{ (1-w)^{2n+2} + (1+w)^{2n+2} \right\} w^{2i} dw \\ &= 2^{-2n-3} \int_0^1 2 \sum_{j=0}^{n+1} \binom{2n+2}{2j} w^{2j+2i} dw \\ &= 2^{-2n-3} \sum_{j=0}^{n+1} \frac{(-n-1)_j (-n+\frac{1}{2})_j}{j! (\frac{1}{2})_j (i+j+\frac{1}{2})}. \end{aligned}$$

Thus the integral equals

$$\begin{aligned} 2^{-4m-4n-5} B(m+1, n+2) \sum_{i=0}^m \frac{(-m)_i (n+2)_i}{i! (m+n+3)_i} \sum_{j=0}^{n+1} \frac{(-n-1)_j (-n+\frac{1}{2})_j}{j! (\frac{1}{2})_j (i+j+\frac{1}{2})} \\ = 2^{-4m-4n-5} B(m+1, n+2) S(m, n+1). \end{aligned}$$

The proof is completed by simplifying  $B(m+1, n+2) S(m, n+1)$ .

**Proposition V.2** For  $\alpha > 0$ ,

$$I(2\alpha, 0) = \frac{\pi}{2^{6+8\alpha}} \frac{\Gamma(2\alpha+1)^2}{\Gamma(2\alpha+\frac{3}{2}) \Gamma(2\alpha+\frac{5}{2})}.$$

**Proof** Follow the previous proof from the beginning to equation (6) which is replaced by

$$\begin{aligned} 2^{-8\alpha-2} \int_0^1 \frac{u^2+1}{(1+u)^4} du \int_0^1 y(1-y)^{2\alpha} \left(1 - \left(\frac{1-u}{1+u}\right)^2 y\right)^{2\alpha} dy \\ = 2^{-8\alpha-2} \int_0^1 \frac{u^2+1}{(1+u)^4} du \sum_{i=0}^{\infty} \frac{(-2\alpha)_i}{i!} \left(\frac{1-u}{1+u}\right)^{2i} B(i+2, 2\alpha+1) \\ = 2^{-8\alpha-2} B(2, 2\alpha+1) \sum_{i=0}^{\infty} \frac{(-2\alpha)_i (2)_i}{i! (2\alpha+3)_i} \int_0^1 \frac{u^2+1}{(1+u)^4} \left(\frac{1-u}{1+u}\right)^{2i} du. \end{aligned}$$

The binomial series terminates when  $2\alpha \in \mathbb{Z}_+$ ; otherwise from the asymptotic property of the gamma function it follows that (with some fixed  $m \in \mathbb{Z}_+$  and  $m-2\alpha > 0$ )

$$\begin{aligned} \frac{(-2\alpha)_{m+n}}{(m+n)!} &= \frac{(-2\alpha)_m}{(m+n)!} (m-2\alpha)_n = \frac{(-2\alpha)_m}{m! \Gamma(m-2\alpha)} \frac{\Gamma(m-2\alpha+n)}{\Gamma(m+1+n)} \\ &\sim \frac{(-2\alpha)_m}{m! \Gamma(m-2\alpha)} n^{-2\alpha-1}, (n \rightarrow \infty), \end{aligned}$$

so by the comparison test the series converges for  $0 \leq y \leq 1$  and  $0 \leq u \leq 1$  provided  $\alpha > 0$ , and can be integrated term-by-term. Also  $B(2, 2\alpha + 1) = \frac{1}{(2\alpha+1)(2\alpha+2)}$  With the same argument as in the previous proof, with  $n = 0$  we obtain

$$\begin{aligned} \int_0^1 \frac{u^2 + 1}{(1+u)^4} \left( \frac{1-u}{1+u} \right)^{2i} du &= \frac{1}{8} \left( \frac{1}{i + \frac{1}{2}} + \frac{1}{i + \frac{3}{2}} \right) = \frac{(i+1)}{4 \left( i + \frac{1}{2} \right) \left( i + \frac{3}{2} \right)} \\ &= \frac{(i+1)! \left( \frac{1}{2} \right)_i}{4i! \left( \frac{1}{2} \right)_{i+2}} = \frac{(2)_i \left( \frac{1}{2} \right)_i}{3 (1)_i \left( \frac{5}{2} \right)_i}. \end{aligned}$$

Then

$$I(2\alpha, 0) = \frac{2^{-8\alpha-2}}{3(2\alpha+1)(2\alpha+2)} \sum_{i=0}^{\infty} \frac{(-2\alpha)_i (2)_i (2)_i \left( \frac{1}{2} \right)_i}{i! (2\alpha+3)_i (1)_i \left( \frac{5}{2} \right)_i}.$$

This is a very-well-poised  ${}_4F_3$  series which is summable using the Rogers-Dougall formula (see [19, 16.4.9]):

$$\begin{aligned} {}_5F_4 \left( \begin{matrix} a, \frac{a}{2} + 1, b, c, d \\ \frac{a}{2}, a - b + 1, a - c + 1, a - d + 1 \end{matrix}; 1 \right) \\ = \frac{\Gamma(a - b + 1) \Gamma(a - c + 1) \Gamma(a - d + 1) \Gamma(a - b - c - d + 1)}{\Gamma(a + 1) \Gamma(a - b - c + 1) \Gamma(a - b - d + 1) \Gamma(a - c - d + 1)}, \end{aligned}$$

the sum converges if one of  $b, c, d$  is a negative integer and it terminates or  $b + c + d - a < 1$ . The formula applies to our sum with  $a = 2, b = -2\alpha, c = \frac{1}{2}, d = \frac{3}{2}$  (that is,  $d = a - d + 1$ ), and  $b + c + d - a = -2\alpha < 1$ . The result is

$$\begin{aligned} I(2\alpha, 0) &= \frac{2^{-8\alpha-2}}{3(2\alpha+1)(2\alpha+2)} \frac{\Gamma(2\alpha+3) \Gamma\left(\frac{3}{2}\right) \Gamma\left(\frac{5}{2}\right) \Gamma(2\alpha+1)}{\Gamma(3) \Gamma\left(2\alpha+\frac{3}{2}\right) \Gamma\left(2\alpha+\frac{5}{2}\right) \Gamma(1)} \\ &= \frac{2^{-8\alpha-6}\pi}{(2\alpha+1)(2\alpha+2)} \frac{\Gamma(2\alpha+3)\Gamma(2\alpha+1)}{\Gamma\left(2\alpha+\frac{3}{2}\right) \Gamma\left(2\alpha+\frac{5}{2}\right)} \\ &= \frac{\pi}{2^{6+8\alpha}} \frac{\Gamma(2\alpha+1)^2}{\Gamma\left(2\alpha+\frac{3}{2}\right) \Gamma\left(2\alpha+\frac{5}{2}\right)}. \end{aligned}$$

Of course the two formulas agree when  $2\alpha \in \mathbb{Z}_{\geq 0}$ .

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